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COMMUNICATION TO THE EXAMINER

Assistant Commissioner for Patents
Washington, D.C. 20231

Sir:

An English language translation of the priority document (Japanese Patent Application Laid-Open 6-251125) is enclosed herewith.

Respectfully submitted,

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CERTIFICATION

I, Takao Kohno; 4-3, Tsuriganecho 2-chome, Chuo-ku, Osaka 540, Japan, hereby certify that I am the translator of the documents in respect of an application for a patent filed in Japan on the 22nd day of February, 1993 (Japanese Patent Application No.5-56582, Laid-Open No.6-251125)

and certify that the following is a true and correct translation to the best of my knowledge and belief.

KOHNO PATENT OFFICE

KOHNO Takao

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(11) Patent Application Laid-Open No.6-251125

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[TITLE OF THE INVENTION] SIGHT LINE/RAY DIRECTION CHANGING DEVICE USED IN DISPLAYING THREE-DIMENSIONAL MOLECULAR INFORMATION

[ABSTRACT] To make it possible to easily grasp the changing operation method and changing operation results when changing a sight line direction and a direction of incidence of parallel rays with respect to three-dimensional molecular information. [CONSTITUTION] A sight line vector initial value setting unit 2 and a ray vector initial value setting unit 3 set a sight line vector initial value and a ray vector initial value, and a ray setting celestial sphere display data initial value setting unit 4 and a sight line setting celestial sphere display data initial value setting unit 5 set initial values of display data for a sight line setting celestial sphere and a ray setting celestial sphere. A sight line setting celestial sphere display processing unit 6 displays a sight line setting celestial sphere to be overlaid on a molecular skeleton, and changes the sight line direction in an interactive manner. A ray setting

celestial sphere display processing unit 7 displays a ray setting celestial sphere to be overlaid on a molecular skeleton and interactively changes the direction of incidence of parallel rays. A geometric conversional information/ray direction conversional information generating unit 8 generates rotational information of the sight line setting celestial sphere and the molecular skeleton, and ray direction conversional information based on change information of a sight line vector and a ray vector.

[WHAT IS CLAIMED IS:]

[Claim 1] A sight line direction changing device used in displaying three-dimensional molecular information, which three-dimensionally displays, on a graphic display, three-dimensional molecular information including a physical quantity obtained from a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton, comprising a sight line setting celestial sphere display processing unit which displays a sight line setting celestial sphere formed of a wireframe model sphere expressing positional information of an observing point and a fixation point on the graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes the sight line direction.

[Claim 2] The sight line direction changing device used in displaying three-dimensional molecular information according to Claim 1, wherein said sight line setting celestial sphere display processing unit changes a shape of a pointer expressing a position of an observing point on said sight line setting celestial sphere before changing the sight line direction so that a three-dimensional position of the observing point in a virtual three-dimensional space on the graphic display can be easily grasped.

[Claim 3] A ray direction changing device used in displaying three-dimensional molecular information, which three-dimensionally displays, on a graphic display, three-dimensional molecular information including a physical quantity obtained through a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton comprising:

a ray setting celestial sphere display processing unit which displays a ray setting celestial sphere formed of a wireframe model sphere expressing the directions of incidence of parallel rays on a graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes the directions of incidence of parallel rays.

[Claim 4] The ray direction changing device used in displaying three-dimensional molecular information according to Claim 3, wherein said ray setting celestial sphere display processing unit changes a shape of a pointer expressing the directions of incidence of parallel rays on said ray setting celestial sphere so that the three-dimensional position of the pointer in a virtual three-dimensional space on the graphic display is easily grasped.

[Claim 5] A sight line/ray direction changing device used in displaying three-dimensional molecular information, which three-dimensionally displays, on a graphic display, three-dimensional molecular information including a physical quantity obtained through a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton, comprising:

a sight line setting celestial sphere display processing unit which displays a sight line setting celestial sphere formed of a wireframe model sphere expressing positional information of an observing point and a fixation point on the graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes a sight line direction; and

a ray setting celestial sphere display processing unit which

displays a ray setting celestial sphere formed of a wireframe model sphere expressing directions of incidence of parallel rays on the graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes the directions of incidence of parallel rays.

[Claim 6] The sight line/ray direction changing device used in displaying three-dimensional molecular information according to Claim 5, wherein said sight line setting celestial sphere display processing unit changes a shape of a pointer expressing a position of an observing point on said sight line setting celestial sphere when changing the sight line direction so that a three-dimensional position of the pointer in a virtual three-dimensional space on the graphic display is easily grasped, and said ray setting celestial sphere display processing unit changes a shape of a pointer expressing directions of incidence of parallel rays on said ray setting celestial sphere so that the three dimensional position of the pointer in a virtual three-dimensional space on the graphic display is easily grasped when changing the directions of incidence of parallel rays.

[DETAILED DESCRIPTION OF THE INVENTION]

[0001]

[Field of Industrial Application] The present invention relates

to a sight line/ray direction changing device used in displaying three-dimensional molecular information, more specifically, a sight line/ray direction changing device used in displaying three-dimensional molecular information by which, when three-dimensionally displaying and analyzing three-dimensional molecular information including a physical quantity obtained through a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton on a graphic display, changes in a sight line direction and directions of incidence of parallel rays are more easily made.

[0002]

[Prior Art] For understanding molecular properties and reactivity, it has been generally known that the results of analyses of molecular orbital calculation and molecular dynamics calculation are very useful. These results of analysis are obtained as a mass of numeral information. Therefore, arts for visualizing such a mass of numeral information as three-dimensional molecular information has become important (for example, refer to Japanese Unexamined Patent Publications No. 61-233872 and No. 64-84392). Based on this visualized three-dimensional molecular information, physical properties based on the molecular three-dimensional structure can be grasped. This three-dimensional molecular information is

displayed in a virtual three-dimensional space on a graphic display.

[0003] For efficient analysis of three-dimensional information on a graphic display, it is necessary that changes in a sight line direction and directions of incidence of parallel rays relating to a virtual three-dimensional space on the graphic display are easily made. Furthermore, it is required that the method of such an operation and operation results can be easily grasped.

[0004] Currently, in most cases, a dial or a slider displayed on a graphic display is used for changing the sight line direction and directions of incidence of parallel rays of three-dimensional molecular information displayed on the graphic display, and rotational information and movement information relating to a virtual three-dimensional space on the graphic display are adapted to them. In this method, it is difficult to grasp the virtual three-dimensional space on the graphic display, and in most cases, an operator is forced to perform the operations depending on his sense.

[0005] There is a case where changes in a sight line direction and directions of incidence of parallel rays are made by using a mouse, however, most such cases involve operations depending on an operator's sense, because three-dimensional operation

is carried out on a graphic display.

[0006]

[Problems to be Solved by the Invention] In the abovementioned conventional sight line/ray direction changing method adopted in displaying of three-dimensional molecular information, when changing a sight line direction and directions of incidence of parallel rays of three-dimensional molecular information displayed on a graphic display, it is always necessary that a virtual three-dimensional space on the graphic display is supposed, however, it is difficult to directly operate rotational information and movement information in a virtual three-dimensional space on the graphic display to change a sight line direction and directions of incidence of parallel rays, and to suppose the results of this operation. Also, in a case where three-dimensional operation is carried out on a graphic display that is a two-dimensional plane, the same problem arises since it is necessary to suppose a virtual three-dimensional space on the graphic display.

[0007] In view of the abovementioned circumstances, an object of the invention is to provide a sight line direction changing device in displaying of three-dimensional molecular information, wherein, when a sight line direction with respect to three-dimensional molecular information displayed on a

graphic display is changed, a wireframe model sphere expressing positional information of an observing point and a fixation point is used so that an operation method and operation results of changes in a sight line direction are easily grasped.

[0008] Another object of the invention is to provide a ray direction changing device used in displaying three dimensional molecular information wherein, when the directions of incidence of parallel rays with respect to three-dimensional molecular information displayed on a graphic display are changed, a wireframe model sphere expressing directions of incidence of parallel rays is used so that an operation method and operation results in changes in directions of the incidence of parallel rays.

[0009] Furthermore, still another object of the invention is to provide a sight line/ray direction changing device constructed so that, when the sight line direction and directions of incidence of parallel rays with respect to three-dimensional molecular information displayed on a graphic display are changed, an operation method and operation results thereof are easily grasped.

[0010]

[Means for Solving Problems] The sight line direction changing device used in displaying three-dimensional molecular

information according to the invention, which three-dimensionally displays, on a graphic display, three-dimensional molecular information including a physical quantity obtained through a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton, comprises a sight line setting celestial sphere display processing unit which displays a sight line setting celestial sphere formed of a wireframe model sphere expressing positional information of an observing point and a fixation point on the graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes the sight line direction.

[0011] Furthermore, the ray direction changing device used in displaying three-dimensional molecular information according to the invention, which three-dimensionally displays, on a graphic display, three-dimensional molecular information including a physical quantity obtained through a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton, comprises a ray setting celestial sphere processing unit which displays a ray setting celestial sphere formed of a wireframe model sphere expressing directions of incidence of parallel rays on the graphic display for displaying three-dimensional molecular information in an overlapping

manner, and interactively changes directions of incidence of parallel rays.

[0012] Furthermore, the sight line/ray direction changing device used in displaying three-dimensional molecular information according to the invention, which three-dimensionally displays, on a graphic display, three dimensional molecular information including a physical quantity obtained through a molecular skeleton and a molecular orbital calculation corresponding to the molecular skeleton, comprises a sight line setting celestial sphere display processing unit which displays a sight line setting celestial sphere formed of a wireframe model sphere expressing positional information of an observing point and a fixation point on the graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes a sight line direction, and a ray setting celestial sphere display processing unit which displays a ray setting celestial sphere formed of a wireframe model sphere expressing directions of incidence of parallel rays on the graphic display for displaying three-dimensional molecular information in an overlapping manner, and interactively changes the directions of incidence of parallel rays.

[0013]

[Embodiments] Next, the present invention is described in detail with reference to the accompanying drawings.

[0014] Fig. 1 is a block diagram showing the construction of a sight line/ray direction changing device in displaying of three-dimensional molecular information relating to an embodiment of the invention. The sight line/ray direction changing device used in displaying three-dimensional molecular information of the present embodiment has a main section comprising a molecular coordinate input unit 1, sight line vector initial value setting unit 2, ray vector initial value setting unit 3, sight line setting celestial sphere display information initial value setting unit 4, ray setting celestial sphere display information initial value setting unit 5, sight line setting celestial sphere display processing unit 6, ray setting celestial sphere display processing unit 7, geometric conversional information/ray direction conversional information generating unit 8, geometric information generating unit 9, and display processing unit 10.

[0015] Referring to Fig. 2, processing of the sight line setting celestial sphere display processing unit 6 comprises a sight line setting celestial sphere display switch judging step 21, sight line setting celestial sphere display erasing step 22, sight line setting celestial sphere pointer existence judging

step 24, pointer display processing step 25, sight line vector change information acquiring step 26, sight line setting celestial sphere parallel movement judging step 27, previous sight line setting celestial sphere display erasing step 28 and sight line setting celestial sphere display information changing step 29.

[0016] Referring to Fig. 3, processing of the ray setting celestial sphere display processing unit 7 comprises ray setting celestial sphere display switch judging step 31, ray setting celestial sphere display erasing step 32, ray setting celestial sphere display information acquiring step 33, ray setting celestial sphere pointer existence judging step 34, pointer display processing step 35, ray vector change information acquiring step 36, ray setting celestial sphere parallel movement judging step 37, previous ray setting celestial sphere display erasing step 38, and ray setting celestial sphere display information changing step 39.

[0017] Fig. 4(a) shows wireframe model spheres expressing information on a sight line direction and directions of incidence of parallel rays to be displayed on a graphic display for displaying three-dimensional molecular information in an overlapping manner. Hereinafter, these two spheres are referred to as a sight line setting celestial sphere S1 and a ray setting

celestial sphere S2. The term sight line indicates a line connecting an observing point (a point from which an object is observed) and a fixation point (a point of an object to be gazed at). The center of the sight line setting celestial sphere S1 expresses the fixation point. Before changing the sight line direction, the sight line is perpendicular to the display screen, and the sight line direction is the direction toward the opposite side of the display screen. The sight line direction always finally returns to this condition.

[0018] The directions of incidence of parallel rays are, as shown in Fig. 4(a), expressed by the directions from the cross-shaped pointer P2 on the ray setting celestial sphere S2 toward the center of the ray setting celestial sphere S2. At the time point at which the molecular skeleton M is displayed initially, the center of the sight line setting celestial sphere S1 and the center of ray setting celestial sphere S2 match each other, and are set as the center of gravity of the molecule. The initial values of the sight line direction and the directions of incidence of parallel rays are set based on a range occupied by the molecular skeleton M in the virtual three-dimensional space on the graphic display.

[0019] Furthermore, in a case where a cross-shaped pointer P1 is displayed on the sight line setting celestial sphere S1,

as shown in Fig. 4(a) and Fig. 4(b), the shape of the pointer P1 is changed depending on the position of the pointer P1 on the sight line setting celestial sphere S1 to express a three-dimensional position in the virtual three-dimensional space on the graphic display.

[0020] To change the sight line direction, two methods are employed. One method is a method for changing the observing point, and as shown as a state [Before moving] (left section) in Fig. 4(b), a position from which it is desired to view the molecular skeleton M as an object is specified to the pointer P1 on the sight line setting celestial sphere S1. Thereby, the sight line direction is changed to be a direction such as from the pointer P1 toward the center of the sight line setting celestial sphere S1. Thereafter, as shown as a state [After moving] (right section) in Fig. 4(b), the molecular skeleton M and the sight line setting celestial sphere S1 rotate around the center of the sight line setting celestial sphere S1 expressing a fixation point until the sight line becomes perpendicular to the display screen. The other method is a method for moving the fixation point, and as shown as a state [Before moving] (left section) in Fig. 4(c), the fixation point is moved by moving the center of the sight line setting celestial sphere S1. After the center of the sight line setting celestial sphere

is moved, as shown as a state [After moving] (right section) in Fig. 4(c), the molecular skeleton M and sight line setting celestial sphere S1 move until the center of the sight line setting celestial sphere S1 comes to the center of the display screen. In addition, by changing the radius of the sight line setting celestial sphere S1, the molecular skeleton M is scaled up and down.

[0021] To change the directions of incidence of parallel rays, two methods are employed. One method is a method for changing the position of the pointer P2 on the ray setting celestial sphere S2, and the other method is a method for moving the center of the ray setting celestial sphere S2. The difference from the case of the sight ray setting celestial sphere S2 is that the positions of the upper and lower poles of the ray setting celestial sphere S2 are fixed to the upper and lower portions of the display screen. This shows that the positional relationship between the screen projecting three-dimensional molecular information and the directions of incidence of parallel rays are always fixed. Thereby, it becomes possible to automatically direct parallel rays on a position to be gazed at (fixation point) of the molecular skeleton M displayed on the graphic display.

[0022] Next, the operation of the sight line/ray direction

changing device thus constructed in displaying of three-dimensional molecular information according to the present embodiment is described.

[0023] The molecular coordinate input unit 1 executes processing for acquiring molecular coordinate information that becomes necessary to display the molecular skeleton M from the results of molecular orbital calculation or molecular dynamics calculation.

[0024] The sight line vector initial value setting unit 2 sets an initial value of the sight line vector (directed vector for determining the sight line direction) to be used for the initial display on the graphic display. The initial value of the sight line vector is calculated and set so that the observing point is positioned so as to realize easier observation of the molecular skeleton M from the range occupied by the molecular skeleton M in the virtual three-dimensional space on the graphic display with a fixation point set at the center of gravity of the molecule.

[0025] The ray vector initial value setting unit 3 sets an initial value of the ray vector (directed vector for determining the directions of incidence of parallel rays). The ray vector initial value is calculated and set so as to have a predetermined angle with respect to the initial value of the sight line vector set

by the sight line vector initial value setting unit 2.

[0026] The sight line setting celestial sphere display information initial value setting unit 4 sets initial values of the sight line setting celestial sphere S1 to be displayed on the graphic display. The sight line setting celestial sphere S1 has data of the same number of dimensions as that of the molecular coordinate information to be displayed on the graphic display, and is handled as a sphere in a three-dimensional space. The initial values to be set for the sight line setting celestial sphere S1 are the center coordinates and the radius of the sight line setting celestial sphere in the virtual three-dimensional space on the graphic display. The initial values of the center coordinates of the sight line setting celestial sphere S1 are set as the center of gravity of the molecule, and the radius is set based on the range occupied by the molecular skeleton M in the virtual three-dimensional space on the graphic display.

[0027] The ray setting celestial sphere display information initial value setting unit 5 sets the initial values of the ray setting celestial sphere S2. The ray setting celestial sphere S2 has two-dimensional information as data, and is positioned on a screen on which the molecular skeleton M in the three-dimensional space is projected. The radius of the ray setting celestial sphere S2 is set so as to be larger than the

radius of a sphere that is formed when the sight line setting celestial sphere S1 is projected on the screen for projecting the molecular skeleton M on. Initial values are set so that the center of the ray setting celestial sphere S2 matches the center of the sight line setting celestial sphere S1 (corresponding to the center of gravity of the molecule) projected on the screen that projects on which the molecular skeleton M is projected. In the case of the ray setting celestial sphere S2, an initial value of the position of the pointer P1 on the ray setting celestial sphere S2, which shows the directions of incidence of parallel rays, is also set. This value is calculated from the ray vector the initial value of which has been set by the ray vector initial value setting unit 3.

[0028] The sight line setting celestial sphere display processing unit 6 judges ON or OFF of the sight line setting celestial sphere display switch (step 21). The sight line setting celestial sphere display switch is turned on to change the sight line direction by using the sight line setting celestial sphere S1, and the initial value thereof is OFF.

[0029] When the sight line setting celestial sphere display switch is OFF, the sight line setting celestial sphere display processing unit 6 executes erase processing of the sight line

setting celestial sphere S1 displayed on the graphic display (step 22). In a case where no sight line setting celestial sphere S1 is displayed on the graphic display, no processing is executed and the process is ended.

[0030] When the sight line setting celestial sphere display switch is ON, the sight line setting celestial sphere display processing unit 6 judges whether or not the pointer P1 exists on the sight line setting celestial sphere S1 (step 24), and in a case where the sight line direction is to be changed, a mouse cursor is positioned on the sight line setting celestial sphere S1, so that display processing of the pointer P1 in accordance with the position of the mouse cursor is executed (step 25). The shape of the pointer P1 on the sight line setting celestial sphere S1 is changed so that the three-dimensional position in the virtual three-dimensional space on the graphic display is easily grasped as shown in Fig. 4(a) and Fig. 4(b).

[0031] Transformation of the pointer P1 is achieved by changing three variables dx, dy, and dφ shown in Fig. 5(a). The reference symbols 2A shown in Fig. 5(a) show the lengths of two line segments forming the pointer P1.

[0032] To determine the variables dx, dy, and dφ, it is supposed that the normal vector at coordinates corresponding to the position of the pointer on the display screen on the sight line

setting celestial sphere S1 is defined as β. As shown in Fig. 5(b), the angle of this normal vector β to the normal vector α of the screen projecting the molecular skeleton M is defined as θ. The vector obtained by projecting the normal vector β on the screen is defined as β'. In this case, the angle between the X axis and the vector β' on the screen is defined as φ. The direction of the X axis defined on the screen corresponds to the horizontal direction on the display screen, and the Y axis corresponds to the vertical direction.

[0033] The variables dx, dy, and dφ are determined as the following formulas by using the variables θ and φ. Herein, A shows a half the length of the two segments forming the pointer P1.

[0034] $dx = A \cdot \sin\theta \cdot \cos\varphi$

$dy = A \cdot \sin\theta \cdot \sin\varphi$

$0° < \varphi \leq 45° \rightarrow d\varphi = \varphi$

$45° < \varphi \leq 135° \rightarrow d\varphi = 90° - \varphi$

$135° < \varphi \leq 225° \rightarrow d\varphi = \varphi - 180°$

$225° < \varphi \leq 315° \rightarrow d\varphi = 270° - \varphi$

$315° < \varphi \leq 360° \rightarrow d\varphi = \varphi - 360°$

[0035] An example of transformation of the pointer P1 is illustrated in Fig. 5(c).

[0036] Subsequently, the sight line setting celestial sphere

display processing unit 6 executes processing for recognizing that the sight line vector has been changed after carrying out an operation for setting the mouse cursor on the sight line setting celestial sphere S1 and pressing the mouse button (step 26). In a case where the sight line vector has been changed, the change information is acquired, and the process is advanced to the next processing. In a case where no change has been made, the process is advanced to the next processing without executing any processing.

[0037] Next, the sight line setting celestial sphere display processing unit 6 judges whether or not the center of the sight line setting celestial sphere S1 has moved in parallel in accordance with the movement of the fixation point (step 27), and when the center of the sphere has moved, erase processing of the sight line setting celestial sphere S1 previously displayed on the graphic display is executed in order to move the sight line setting celestial sphere S1 in parallel to the molecular skeleton M (step 28). When no sight line setting celestial sphere S1 is displayed on the display screen, the process is ended without executing any processing.

[0038] Subsequently, the sight line setting celestial sphere display processing unit 6 executes processing for generating display information of the sight line setting celestial sphere

S1 in which sight line vector change information has been reflected when the sight line setting celestial sphere S1 has been moved in parallel (step 29). Display information to be generated includes the coordinates of the center of the sight line setting celestial sphere S1 and the radius thereof in the virtual three-dimensional space on the graphic display.

[0039] Next, the ray setting celestial sphere display processing unit 7 judges ON or OFF of the ray setting celestial sphere display switch (step 31). The ray setting celestial sphere display switch is a switch which is turned on to change the directions of incidence of parallel rays by using the ray setting celestial sphere S2, and the initial value of the switch is OFF.

[0040] When the ray setting celestial sphere display switch is OFF, the ray setting celestial sphere display processing unit 7 executes erase processing of the ray setting celestial sphere S2 displayed on the graphic display (step 32). In a case where no ray setting celestial sphere S2 is displayed on the graphic display, the process is ended without executing any processing.

[0041] When the ray setting celestial sphere display switch is ON, the ray setting celestial sphere display processing unit 7 calculates the position of the pointer P2 showing the

directions of incidence of parallel rays on the ray setting celestial sphere S2 and the center position of the ray setting celestial sphere S2 from parallel ray information at a time point of passing through the processing of this processing unit (step 33). In a case of passing through this processing for the first time, initial values of display information of the ray setting celestial sphere S2 set by the ray setting celestial sphere display information initial value setting unit 5 are set. In other cases, the position of the pointer P2 showing the directions of incidence of parallel rays on the ray setting celestial sphere S2 and the center position of the ray setting celestial sphere S2 are calculated from parallel ray information set by the geometric conversional information/ray direction conversional information generating unit 8.

[0042] Next, the ray setting celestial sphere display processing unit 7 judges whether or not the pointer P2 exists on the ray setting celestial sphere S2 (step 34), and to change the directions of incidence of parallel rays, a mouse cursor is positioned on the ray setting celestial sphere S2, and display processing of the pointer P2 in accordance with the mouse cursor position is executed (step 35). The shape of the pointer P2 on the ray setting celestial sphere S2 is changed, as shown in Fig. 4(a) and Fig. 4(b), so that the three-dimensional

position in the virtual three-dimensional space on the graphic display can be grasped easily as is the case with the shape of the pointer P1 on the sight line setting celestial sphere S1.

[0043] Subsequently, the ray setting celestial sphere display processing unit 7 executes processing for recognizing that the ray vector has been changed when an operation for setting the mouse cursor on the ray setting celestial sphere S2 and pressing the mouse button has been carried out (step 36). When the ray vector has been changed, information on this change is acquired, and the process is advanced to the next processing. When no change has been made, the process is ended without executing any processing.

[0044] Next, the ray setting celestial sphere display processing unit 7 judges whether or not the center of the ray setting celestial sphere S2 has been moved in parallel (step 37), and when the sphere has been moved in parallel, executes erase processing of the ray setting celestial sphere S2 previously displayed on the graphic display in order to move the ray setting celestial sphere S2 in parallel to the molecular skeleton M (step 38). When no ray setting celestial sphere S2 is displayed on the display screen, the process is advanced to the next processing without executing any processing. When the parallel

movement has not been made, the process is ended without executing any processing.

[0045] Subsequently, the ray setting celestial sphere display processing unit 7 executes processing for generating display information of the ray setting celestial sphere S2 in which ray vector change information has been reflected when the ray setting celestial sphere S2 has been moved in parallel (step 39). Display information to be generated includes the coordinates of the center of the ray setting celestial sphere S2 and the radius thereof in the virtual three-dimensional space on the graphic display.

[0046] The geometric conversional information/ray direction conversional information generating unit 8 generates rotational information for rotating the sight line setting celestial sphere S1 and the molecular skeleton M so that the sight line vector becomes perpendicular to the display screen based on the sight line vector change information. Furthermore, the geometric conversional information/ray direction conversional information generating unit 8 generates conversional information for changing the directions of incidence of parallel rays based on the ray vector change information. Even when only the sight line vector has been changed, ray vector conversional information for setting a ray

vector having an appropriate angle with this sight line vector is generated.

[0047] The geometric information generating unit 9 generates geometric information that is necessary for displaying the molecular skeleton M and the sight line setting celestial sphere S1 based on the molecular coordinate information, sight line setting celestial sphere display information, rotating operation information and parallel ray information. In addition, the geometric information generating unit 9 generates geometric information that is necessary for displaying the sight line setting celestial sphere S2 and displaying the pointer P2 showing the directions of incidence of parallel rays based on the ray setting celestial sphere display information.

[0048] The display processing unit 10 executes display processing on the graphic display based on the geometric information. After the display processing based on the geometric information, the display processing unit 10 turns the control back to the sight line setting celestial sphere display processing unit 6, and then processing of the sight line setting celestial sphere display processing unit 6, ray setting celestial sphere display processing unit 7, geometric conversional information/ray direction conversional information generating unit 8, geometric information

generating unit 9, and display processing unit 10 is repeated.

[0049]

[Effects of the Invention] As described above, according to the invention, in a case where a sight line direction is changed with respect to three-dimensional molecular information displayed on a graphic display, a sight line setting celestial sphere formed of a wireframe model sphere expressing positional information of an observing point and a fixation point is displayed, whereby it becomes easier to grasp a virtual three-dimensional space on the graphic display, and it becomes possible to easily grasp an operation method for changing the sight line direction and operation results.

[0050] Furthermore, according to the invention, in a case where the directions of incidence of parallel rays are changed with respect to three-dimensional molecular information displayed on a graphic display, a ray setting celestial sphere formed of a wireframe model sphere expressing the directions of incidence of parallel rays is displayed, whereby it becomes easier to grasp a virtual three-dimensional space on the graphic display, and it becomes possible to easily grasp an operation method for changing the directions of incidence of parallel rays and operation results.

[0051] Moreover, according to the invention, in a case where

a sight line direction is changed with respect to three-dimensional molecular information displayed on a graphic display, a sight line setting celestial sphere formed of a wireframe model sphere expressing positional information of an observing point and a fixation point and a ray setting celestial sphere formed of a wireframe model sphere expressing the directions of incidence of parallel rays are displayed, whereby it becomes easier to grasp a virtual three-dimensional space on the graphic display, and it becomes possible to easily grasp operation methods for changing the sight line direction and the directions of incidence of parallel rays and operation results.

[BRIEF DESCRIPTION OF THE DRAWINGS]

[Fig. 1] is a block diagram showing the construction of the sight line/ray direction changing device used in displaying three-dimensional molecular information relating to an embodiment of the invention.

[Fig. 2] is a flowchart showing processing of the sight line setting celestial sphere display processing unit in Fig. 1.

[Fig. 3] is a flowchart showing processing of the ray setting celestial sphere display processing unit in Fig. 1.

[Figs. 4] (a) is a drawing showing a display example of the observing point setting celestial sphere and the ray setting

celestial sphere to be used for changing the sight line direction and the directions of incidence of parallel rays; (b) is a drawing illustrating the rotation process of the observing point setting celestial sphere and the molecular skeleton in a case where the sight line direction has been changed; and (c) is a drawing illustrating the movement process of the sight line setting celestial sphere and the molecular skeleton when the fixation point has been moved.

[Figs. 5] (a) is an explanatory view of variables to be used for transformation of the pointer; (b) is an explanatory view of a vector to be used for transformation of the pointer; and (c) is a drawing showing an example of transformation of the pointer.

[Description of Symbols]

1 Molecular coordinate input unit

2 Sight line vector initial value setting unit

3 Ray vector initial value setting unit

4 Sight line setting celestial sphere display information initial value setting unit

5 Ray setting celestial sphere display information initial value setting unit

6 Sight line setting celestial sphere display processing unit

7 Ray setting celestial sphere display processing unit

8 Geometric conversional information/ray direction conversional information generating unit

9 Geometric information generating unit

10 Display processing unit

21 Sight line setting celestial sphere display switch judging step

22 Sight line setting celestial sphere display erasing step

24 Sight line setting celestial sphere pointer existence judging step

25 Pointer display processing step

26 Sight line vector change information acquiring step

27 Sight line setting celestial sphere parallel movement judging step

28 Previous sight line setting celestial sphere display erasing step

29 Sight line setting celestial sphere display information changing step

31 Ray setting celestial sphere display switch judging step

32 Ray setting celestial sphere display erasing step

33 Ray setting celestial sphere display information acquiring step

34 Ray setting celestial sphere pointer existence judging

step

35 Pointer display processing step

36 Ray vector change information acquiring step

37 Ray setting celestial sphere parallel movement judging step

38 Previous ray setting celestial sphere display erasing step

39 Ray setting celestial sphere display information changing step

M Molecular skeleton

P1 Sight line setting pointer

P2 Ray setting pointer

S1 Sight line setting celestial sphere

S2 Ray setting celestial sphere